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NiFe/Cr/NiFe 薄膜之電子結構與磁性研究

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X-ray absorption spectroscopy (XAS) is well established as a suitable tool for investigating the electronic structure and local atomic environment. Near edge x-ray absorption fine structure (NEXAFS), which is also sometimes referred to as x-ray absorption near edge structure (XANES) spectroscopy is very sensitive to the chemical bonding in the material, which arises from the dipole electronic transitions from core states of the absorbing atom that have well-defined orbital angular momentum into empty electronic states above the Fermi level. The strength of extended x-ray absorption fine structure (EXAFS) spectroscopy is its ability to provide structural information on systems that cannot be studied with other conventional techniques. It is the appropriate tool to determine the local structure and the type of neighbors. EXAFS spectra contain information about the interatomic distance and coordination numbers.

Rare-earth based manganite perovskites

Recently, electron-doped lanthanum manganites have attracted much interest due to the exhibition of interesting novel properties. The fundamental origins of these properties still remain controversial. Electron doped manganites finds application in device fabrication along with hole doped one. The size of the substituting cation is found to influence on structural, magnetic and electrical properties of the material. Further, knowledge of the valence of Mn ions and interactions between various atoms in the material is essential to elucidate the origins of the exhibited anomalous properties. The partial substitution of La ions by Pr ions is of special interest, since the resultant narrow-gap CMR compounds possess an interesting phase diagram. Therefore we performed XANES and EXAFS studies on a typical electron doped lanthanum manganite perovskite, $(La_{1-x}Pr_x)_{0.85}Zr_{0.15}MnO_3$ with x = 0.05, 0.1, 0.15 and 0.2 as an attempt to resolve the controversy regarding the fundamental origins of the exhibited anomalous properties.

An analysis of Mn $L_{3,2}$-, O *K*- and Pr $M_{5,4}$-edge XANES spectra demonstrate that the substitution of smaller ionic radii Pr for La changes O 2*p*-Mn 3*d* and O 2*p*-Pr 4*f* hybridized states. The O 2*p*-Mn 3*d* variations will affect the electronic states near the Fermi level. The Pr substitution is observed to increase the average effective positive charge on the Mn ion, which is argued to either potentially create polaronic distortions in the material or to cause a JT distortion around the Mn site. These distortions may alter the magneto resistance of the material. The EXAFS analysis clearly shows changes to the local atomic structure around the Mn atom caused by Pr substitution. Overall, XANES and EXAFS analysis revealed a reduced distortion in the MnO_6 octahedron or a local disorder in the lattice, which may be caused by the localization of charge carriers and/or an increase in the average effective positive charge on the Mn ions.

Semiconductor nanorods and Diamond like carbon films

ZnO nanorods and nanowires are particularly interesting because they can be used to tune electronic and optoelectronic devices that involve UV lasing action. Knowledge of the electronic structure of the nanorods is crucial to understand the basic physics for these applications. Hence we performed x-ray absorption studies on ZnO nanorods of various diameters of ~150±40, 80±20 and 45±10nm to find the diameter dependence on the electronic structure. An analysis of O *K*-, Zn L_3- and *K*-edges XANES spectra revealed increased numbers of O 2*p* and Zn 4*p* unoccupied states with the downsizing of the nanorods that reflects the enhancement of surface states when the diameter is decreased. Valence-band photoemission spectra showed a significant narrowing of the valence band for the 45nm diameter nanorod. The Zn 3*d* intensities in the scanning photoelectron microscopy (SPEM) spectra are drastically reduced for all nanorods as compared to ZnO reference film, which can be interpreted as a reduction in density of itinerant final states or in transition probability.

Some other collaborative research were also carried out on different materials such as $Ba_{1-x}Sr_xTiO_3$, $Pb_{1-x}Sr_xTiO_3$, hydrogenated amorphous carbon films, diamond like carbon thin films and silicon doped diamond like carbon thin films. Most of these results are either published or communicated/to be published in international recognized journals.

Presently, we are involved in the study of the electronic structure of diamond like carbon films (DLC) and its effect on ion beam irradiation, a collaborative work with Industrial Technology Research Institute of Taiwan. DLC has considerable technological applications, especially in the field of flat panel displays. Recently, research on this material is revived due to the demonstration that liquid crystal (LC) alignment could be created on any carbonaceous substrate by inducing orientational order at its surface.

XANES spectra of DLC at C *K*- edge and valence band photoemission spectra (PES) at various photon energies were measured to study the electronic structure of this material. X-ray diffraction (XRD) study revealed the samples as amorphous, while Fourier transform infrared (FTIR) spectra was totally different from the one obtained by us on Si-doped hydrogenated amorphous carbon films and showed different transmission bands related to $C\text{-}H_n$ stretching modes, C-H bending mode, C-O bond, C-C mode and C=C bond. Energy dispersive spectra (EDS) of the DLC film showed high percentage of oxygen content in the material, in consistent with the SEM analysis where the presence of atmospheric oxygen in the sample was revealed. C *K*-edge showed a broadened σ^* feature due to the overlapping C 1s to σ^* transitions at sp, sp^2 and sp^3 sites. The second absolute gap was not resolved in DLC film, which may attribute to the high degree of disorder, band tailing and high defect density of states that possibly almost filled up the minimum at that energy. The angle dependent polarized XANES at C K-edge indicated an anisotropy for the π^* resonance intensity with the incident angle of the x-ray photon. The valence band PES mainly showed features predominantly associated with C-C π and σ bond states. The spectra indicated broadening of the π feature and enhancement of the σ feature with an increase of photon energy between 100 and 140 eV.

In order to find the effect of ion beam irradiation on the electronic structure of DLC films, we measured XRD, FTIR, XANES and PES spectra of DLC films deposited at different growth conditions before and after ion beam irradiation at varying hydrogen concentration (10% and 20%). The energy of the irradiation was 500 eV for time duration of 50 seconds at an angle of incidence 20°. Earlier investigations proved that by choosing appropriate ion energies and doses, defects localized in the near surface region with a predetermined disorder level might be readily produced. We are in the process of analyzing the initial results and also intend to measure the angle dependent XANES spectra of DLC films before and after ion beam irradiation. These spectra are expected to give qualitative and quantitative information regarding the orientation of the π states and its dependence on ion beam irradiation. The findings expect industrially useful especially in liquid crystal display industry due to the recent reports where they demonstrated that ion beam irradiation could define the alignment of the rings on the film surface. We also intend to measure the temperature dependent spectra of DLC films to study the effect of temperature on the electronic structure of the sample before and after ion beam irradiation.

List of publications:

- "Effect of the Ca content on the electronic structure of $Pb_{1-x}Ca_xTiO_3$ perovskites". J. C. Jan, K. P. Krishna Kumar, J.W. Chiou, H. M. Tsai. H. L. Shih, H. C. Hsueh, S. C. Ray, K. Asokan, W. F. Pong, M. H. Tsai, S. Y. Kuo and W. F. Hsieh, *Appl. Phys. Lett.*83, 3311 (2003).

- "Effect of Pr substitution on the electronic structure of $(La_{1-x}Pr_x)_{0.85}Zr_{0.15}MnO_3$- K. P. Krishna Kumar, J. C. Jan, J. W. Chiou, H. M. Tsai, C. W. Bao, B. C. Hsu, D. C. Ling and W. F. Pong, and M.-H. Tsai" K. P. Krishna Kumar, J. C. Jan, J. W. Chiou, H. M. Tsai, S. C. Ray, B.C. Hsu, D. C. Ling and W. F. Pong *J. Electr. Spectr. Rel. Phenom.* (2005) (In Press).

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- "X-ray absorption spectroscopy (XAS) study of dip deposited a-C:H(OH) thin films" S. C. Ray, H. M. Tsai, J. W. Chiou, B. Bose, J. C. Jan, Krishna Kumar,W. F. Pong, D. Dasgupta and M.-H. Tsai, *J. Phys.: Condens. Matter* **16,** 5713 (2004).

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